

FILE 'REGISTRY' ENTERED AT 15:33:12 ON 06 NOV 2008

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 6 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 15:34:09 ON 06 NOV 2008

L4 2 S L3

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

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Switching to the Registry File...

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=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:33:12 ON 06 NOV 2008

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STRUCTURE FILE UPDATES: 5 NOV 2008 HIGHEST RN 1070955-84-8

DICTIONARY FILE UPDATES: 5 NOV 2008 HIGHEST RN 1070955-84-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

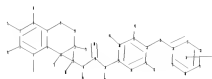
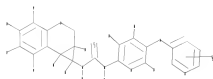
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=>

Uploading C:\Program Files\STNEXP\Queries\10526598amended.str



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chain nodes :
7  8  14 15 16 18 25 33 35 36 37 38 39 40 41 42 43 44
ring nodes :
1  2  3  4  5  6  9 10 11 12 13 19 20 21 22 23 24 26 27 28 29 30
31
chain bonds :
1-7  2-36  3-35  4-8  11-39  12-37  13-14  13-38  14-15  14-40  15-16  15-18  16-19
16-41  20-44  21-43  22-25  23-42  25-26
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-9  6-12  9-10  10-11  11-12  11-13  12-13  19-20
19-24  20-21  21-22  22-23  23-24  26-27  26-31  27-28  28-29  29-30  30-31
exact/norm bonds :
5-9  6-12  9-10  10-11  11-12  11-13  12-13  13-14  14-15  15-16  15-18  16-19
22-25
25-26
exact bonds :
1-7  2-36  3-35  4-8  11-39  12-37  13-38  14-40  16-41  20-44  21-43  23-42
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  19-20  19-24  20-21  21-22  22-23  23-24  26-27  26-31
27-28  28-29  29-30  30-31

```

G1:O,S

G2:H,Cl,Br,F,I,CN

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:Atom 20:Atom
21:Atom 22:Atom
23:Atom 24:Atom 25:CLASS 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
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43:CLASS

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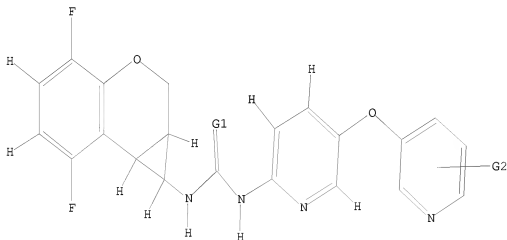
\Rightarrow S 11

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100.0% PROCESSED          0 ITERATIONS          0 ANSWERS
SEARCH TIME: 00.00.01
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L2 0 SEA SSS SAM L1

$$\Rightarrow d_{11}$$

L1 HAS NO ANSWERS
L1 STR



G1 O, S

G2 H, Cl, Br, F, I, CN

Structure attributes must be viewed using STN Express query preparation.

$$\Rightarrow s \perp\!\!\!\perp sss \text{ full}$$

FULL SEARCH INITIATED 15:33:44 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 50 TO ITERATE

100.0% PROCESSED 50 ITERATIONS
SEARCH TIME: 00.00.01

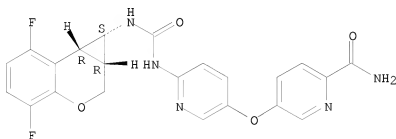
6 ANSWERS

L3 6 SEA SSS FUL L1

=> d l3 scan

L3 6 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Pyridinecarboxamide, 5-[6-[[[(6aR,7S,7aR)-1,4-difluoro-6,6a,7,7a-tetrahydrobenzo[b]cyclopropa[d]pyran-7-yl]amino]carbonyl]amino]-3-pyridinyloxy]-
MF C22 H17 F2 N5 O4

Absolute stereochemistry.

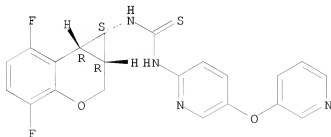


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L3 6 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Thiourea, N-[(6aR,7S,7aR)-1,4-difluoro-6,6a,7,7a-tetrahydrobenzo[b]cyclopropa[d]pyran-7-yl]-N'-[5-(3-pyridinyloxy)-2-pyridinyl]-
MF C21 H16 F2 N4 O2 S

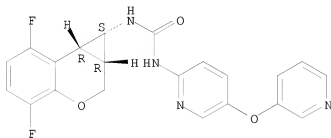
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 6 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Urea, N-[(6aR,7S,7aR)-1,4-difluoro-6,6a,7,7a-
tetrahydrobenzo[b]cyclopropa[d]pyran-7-yl]-N'-[5-(3-pyridinyloxy)-2-
pyridinyl]-
MF C21 H16 F2 N4 O3

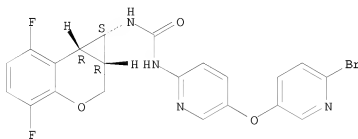
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 6 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Urea, N-[5-[(6-bromo-3-pyridinyl)oxy]-2-pyridinyl]-N'-[(1S,1aR,7bR)-4,7-
difluoro-1,1a,2,7b-tetrahydrobenzo[b]cyclopropa[d]pyran-1-yl]-
MF C21 H15 Br F2 N4 O3

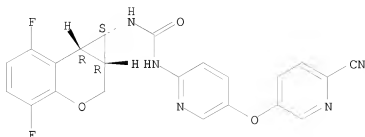
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 6 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Urea, N-[5-[(6-cyano-3-pyridinyl)oxy]-2-pyridinyl]-N'-[(1S,1aR,7bR)-4,7-
difluoro-1,1a,2,7b-tetrahydrobenzo[b]cyclopropa[d]pyran-1-yl]-
MF C22 H15 F2 N5 O3

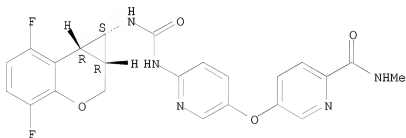
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 6 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Pyridinecarboxamide, 5-[[6-[[[(1S,1aR,7bR)-4,7-difluoro-1,1a,2,7b-
tetrahydrobenzo[b]cyclopropa[d]pyran-1-yl]amino]carbonyl]amino]-3-
pyridinyloxy]-N-methyl-
MF C23 H19 F2 N5 O4

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file hcaplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
178.82	179.03

FILE 'HCAPLUS' ENTERED AT 15:34:09 ON 06 NOV 2008
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FILE COVERS 1907 - 6 Nov 2008 VOL 149 ISS 19
FILE LAST UPDATED: 5 Nov 2008 (20081105/ED)

HCAPLUS now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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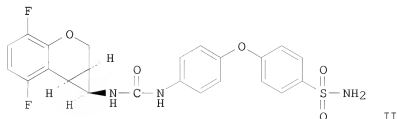
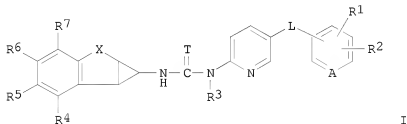
L4 2 L3

=> d l4 1-2 ti abs bib hitstr

L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

TI Preparation of non-nucleotide reverse transcriptase inhibitors

GI



AB Title compds. I [A = CH, N; R1 = SO1-2Ra, CORb, etc.; Ra-b = alkyl, alkoxy, amino, etc.; R2 = H, halo CN, etc.; L = O, SO0-2, CH2; R3 = H,

alkyl; R4-7 = H, alkyl, alkenyl, etc.; X = divalent alkyl; T = O] are prepared For instance, II is prepared in 4 steps from 4-hydroxy-N-(tert-butyl)benzenesulfonamide, 5-bromo-2-nitropyridine and (1S,1aR,7bS)-4,7-difluoro-1,1a,2,7b-tetrahydrocyclopropan[c]chromene-1-carboxylic acid (prior art). II was assayed for HIV activity with an IC50 = 29 nM. I have utility as HIV antivirals.

AN 2005:638849 HCAPLUS <<LOGINID:20081106>>

DN 143:153297

TI Preparation of non-nucleotide reverse transcriptase inhibitors

IN Sund, Christian; Roue, Nathalie; Lindstroem, Stefan; Antonov, Dmitry; Sahlberg, Christer; Jansson, Katarina

PA Medivir AB, Swed.

SO PCT Int. Appl., 118 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005066131	A1	20050721	WO 2004-SE2034	20041230
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	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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	AU 2004312284	A1	20050721		
	CA 2550187	A1	20050721	CA 2004-2550187	20041230
	EP 1701942	A1	20060920	EP 2004-809207	20041230
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	CN 1926108	A	20070307	CN 2004-80042322	20041230
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	JP 2007519640	T	20070719	JP 2006-549182	20041230
	IN 2006DN03577	A	20070831	IN 2006-DN3577	20060621
	MX 2006PA07726	A	20061002	MX 2006-PA7726	20060705
	US 20080070951	A1	20080320	US 2007-584933	20070910
PRAI	SE 2004-21	A	20040108		
	SE 2004-585	A	20040309		
	WO 2004-SE2034	W	20041230		

OS CASREACT 143:153297; MARPAT 143:153297

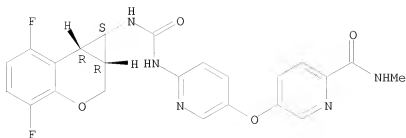
IT 860298-39-1P 860298-41-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted tricyclic non-nucleotide reverse transcriptase inhibitors)

RN 860298-39-1 HCAPLUS

CN 2-Pyridinecarboxamide, 5-[[[6-[[[(1S,1aR,7bR)-4,7-difluoro-1,1a,2,7b-tetrahydrobenzo[b]cyclopropa[d]pyran-1-yl]amino]carbonyl]amino]-3-pyridinyl]oxy]-N-methyl- (CA INDEX NAME)

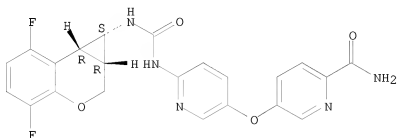
Absolute stereochemistry.



RN 860298-41-5 HCAPLUS

CN 2-Pyridinecarboxamide, 5-[[[6-[[[(6aR,7S,7aR)-1,4-difluoro-6,6a,7,7a-tetrahydrobenzo[b]cyclopropa[d]pyran-7-yl]amino]carbonyl]amino]-3-pyridinyl]oxy]- (CA INDEX NAME)

Absolute stereochemistry.

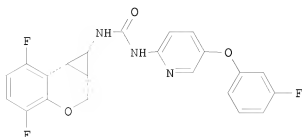
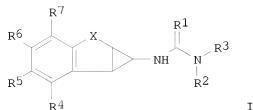


RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

TI Preparation of pyridinyl(thio)urea derivatives of cyclopropachromenes, cyclopropaindenes, cyclopropanaphthalenes, and benzocyclopropacycloheptenes as non-nucleoside reverse transcriptase inhibitors

GI



AB Title compds. I [R1 = O, S; R2 = (substituted) N-containing heterocycle, whose N is located at the 2 position relative to the (thio)urea group; R3 = H, alkyl; R4-R7 = H, alkyl, alkenyl, alkynyl, haloalkyl, alkanoyl, haloalkanoyl, alkoxy, haloalkoxy, alkoxyalkyl, haloalkoxyalkyl, hydroxyalkyl, aminoalkyl, carboxyalkyl, cyanoalkyl, amino, COOH, carbamoyl, cyano, halo, OH, O, etc.; X = (CR8R9)n-D-(CR8R9)m; D = a bond, (substituted)amino, O, S, SO, SO2; R8, R9 = H, alkyl, haloalkyl, OH; R8R9 = O; n, m = 0-2, provided that they are not both 0 when D is a bond] were prepared as non-nucleoside reverse transcriptase inhibitors. Thus, reaction of (1S,1aR,7bS)-4,7-difluoro-1,1a,2,7b-tetrahydrocyclopropa[c]chromene-1-carboxylic acid (preparation given) with 5-(3-fluorophenoxy)-2-aminopyridine yielded compound II.

AN 2004:220140 HCAPLUS <<LOGINID::20081106>>
DN 140:270741

TI Preparation of pyridinyl(thio)urea derivatives of cyclopropachromenes, cyclopropaindenes, cyclopropanaphthalenes, and benzocyclopropacycloheptenes as non-nucleoside reverse transcriptase inhibitors

IN Antonov, Dmitry; Sund, Christian; Lindstroem, Stefan; Sahlberg, Christer
PA Medivir Ab, Swed.

SO PCT Int. Appl., 121 pp.

CODEN: PIXXD2

DT Patent

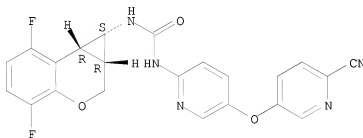
LA English

FAN.CNT 1

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RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,				

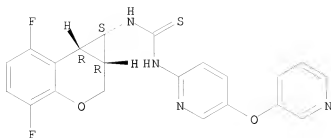
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CN	1694700	A 20051109 CN 2003-824933 20030905
JP	2005538155	T 20051215 JP 2004-533489 20030905
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MX	2005PA02545	A 20050930 MX 2005-PA2545 20050304
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PRAI	EP 2002-19997	A 20020905
IT	WO 2003-EP9872	W 20030905
OS	MARPAT 140:270741	
IT	672946-33-7P	
	RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of pyridinyl(thio)urea derivs. of cyclopropachromenes, cyclopropaindenes, cyclopropanaphthalenes, and benzocyclopropacycloheptenes as non-nucleoside reverse transcriptase inhibitors)	
RN	672946-33-7	HCAPLUS
CN	Urea, N-[5-[(6-cyano-3-pyridinyl)oxyl]-2-pyridinyl]-N'-[(1S,1aR,7bR)-4,7-difluoro-1,1a,2,7b-tetrahydrobenzo[b]cyclopropa[d]pyran-1-yl]- (CA INDEX NAME)	

Absolute stereochemistry.



IT	672946-19-9P 672946-21-3P 672946-31-5P
	RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of pyridinyl(thio)urea derivs. of cyclopropachromenes, cyclopropaindenes, cyclopropanaphthalenes, and benzocyclopropacycloheptenes as non-nucleoside reverse transcriptase inhibitors)
RN	672946-19-9 HCAPLUS
CN	Thiourea, N-[(6aR,7S,7aR)-1,4-difluoro-6,6a,7,7a-tetrahydrobenzo[b]cyclopropa[d]pyran-7-yl]-N'-[5-(3-pyridinyloxy)-2-pyridinyl]- (CA INDEX NAME)

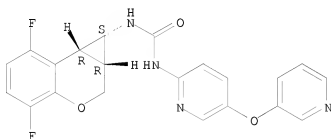
Absolute stereochemistry.



RN 672946-21-3 HCAPLUS

CN Urea, N-[(6aR,7S,7aR)-1,4-difluoro-6,6a,7,7a-tetrahydrobenzo[b]cyclopropa[d]pyran-7-yl]-N'-[5-(3-pyridinyloxy)-2-pyridinyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 672946-31-5 HCAPLUS

CN Urea, N-[5-[(6-bromo-3-pyridinyl)oxy]-2-pyridinyl]-N'-[(1S,1aR,7bR)-4,7-difluoro-1,1a,2,7b-tetrahydrobenzo[b]cyclopropa[d]pyran-1-yl]- (CA INDEX NAME)

Absolute stereochemistry.

